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Connected graphs with maximal Q-index: The one-dominating-vertex case

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ABSTRACT

By the signless Laplacian of a (simple) graph G we mean the matrix $Q(G) = D(G) + A(G)$, where $A(G), D(G)$ denote respectively the adjacency matrix and the diagonal matrix of vertex degrees of G. For every pair of positive integers n, k, it is proved that if $3 \leq k \leq n-3$, then $H_{n,k}$, the graph obtained from the star $K_{1,n-1}$ by joining a vertex of degree 1 to $k+1$ other vertices of degree 1, is the unique connected graph that maximizes the largest signless Laplacian eigenvalue over all connected graphs with n vertices and $n+k$ edges.

1. Introduction

For a (simple) graph G, by the *signless Laplacian* of G we mean the matrix $Q(G) = D(G) + A(G)$, where $A(G), D(G)$ denote respectively the adjacency matrix and the diagonal matrix of vertex degrees of G. The largest eigenvalue (or, equivalently, the spectral radius) of $A(G)$ is usually referred to as the *index* of G.

We are interested in the problem of determining connected graphs (or, not necessarily connected, graphs) that maximize the Q-index (i.e., the largest signless Laplacian eigenvalue or, equivalently,

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the signless Laplacian spectral radius) over all connected graphs (or graphs) with given numbers of vertices and edges. Study of this topic began with the work of Fan [16] in 2004 on the unicyclic case (in the setting of mixed graphs), followed by Fan et al. [17,27] on the bicyclic case and the tricyclic case respectively. Recently Chang and Tam [10] have also determined graphs with maximal Q-index among all graphs with m edges and at most $m - k$ vertices for $k = 0, \ldots, 3$.

The corresponding maximal index problem is an important classic problem in spectral graph theory. Its origin can be traced back to Schwarz's rearrangement theorem (see [25]), which says that *if n^2 nonnegative real numbers (not necessarily pairwise distinct) are given, then the largest spectral radius of a matrix whose entries are these given numbers can be found among those matrices where the entries in each row and each column are non-increasing.* Restricting attention to $(0, 1)$-matrices, in [7] Brualdi and Hoffman considered the problems of determining the maximum spectral radius $\mu_{n,k}$ attainable by a $(0, 1)$-matrix of order n with k 1's and the maximum spectral radius $\sigma_{n,2q}$ attainable by a symmetric $(0, 1)$-matrix of order n with zero trace and $2q$ 1's (i.e., the adjacency matrix of a graph with n vertices and q edges). They found the values of $\mu_{n,k}$ and $\sigma_{n,2q}$ in the cases $k = m^2$, $k = m^2 + 1$, and $q = \binom{m}{2}$, and characterized those matrices achieving the values $\mu_{n,k}$ and $\sigma_{n,2q}$. For the symmetric problem they posed a conjecture, known as the Brualdi–Hoffman conjecture. The conjecture was tackled by Friedland [18,19] and finally settled in the affirmative by Rowlinson [24].

The maximal index problem for the class of connected graphs with n vertices and m edges, treated by a number of researchers, including Brualdi and Solheid [8], Cvetković and Rowlinson [12], Bell [4], Olesky, Roy and Driessche [23], etc., has been solved only for special choices of n and m. (For a description of their results, see [13, p. 72] or [23, Sections 5,6].) Connected with the problem is a well-known conjecture (see [26] or [3]), which roughly says that in each case the optimal graph is one of the (degree) maximal graphs $H_{n,k}$ or $G_{n,k}$. (The definition of $H_{n,k}$ and $G_{n,k}$ will be given later.) Recently, Bhattacharya et al. [5] also studied the maximal index problem for bipartite graphs, where the number of edges and the number of vertices on each side of the bipartition are given. They stated a conjectured solution, which is an analog of the Brualdi–Hoffman conjecture for graphs, and proved the conjecture in some special cases.

In [28, Theorem 5.2] Tam and Wu have proved that for any positive integers n, k with $3 \leq k \leq n-3$, we have $q_1(H_{n,k}) > q_1(G_{n,k})$. We want to point out that the proof as given in [28] contains an error: in one case of the proof, $H_{n,n-3}$ is mistaken as $C(2, n - 2)$ instead of $C(n - 2, 2)$. A correct proof, following the original line of thinking, can be found in Wu's thesis [29].

The following is the main result of this paper:

Theorem. *If $3 \leq k \leq n - 3$, then $H_{n,k}$, the graph obtained from the star $K_{1,n-1}$ by joining a vertex of degree 1 to $k+1$ other vertices of degree 1, is the unique connected graph that maximizes the Q-index over all connected graphs with n vertices and $n + k$ edges.*

We call a vertex of a graph *dominating* if it is adjacent to every other vertex of the graph. Note that a graph of order n with two or more dominating vertices has at least $2n - 3$ edges. So our result settles the one-dominating-vertex case (as well as the case $k = n - 3$) of the maximal Q-index problem for the class of connected graphs with n vertices and $n + k$ edges.

Here we restrict our attention to $k \geq 3$, because for $k = -1, 0, 1$ or 2 — that is, the tree case, the unicyclic case, the bicyclic case and the tricyclic case respectively — the answers to the problem are known: for $k = -1, 0, 1$, $H_{n,k}$ is still the unique optimal graph, noting that $H_{n,-1}$ is equal to the star $K_{1,n-1}$; for $k = 2$, there are two optimal graphs, namely, $H_{n,2}$ and $G_{n,2}$.

This paper is organized as follows. In Section 2 we give relevant definitions and some preparatory results. In Section 3, using line graph as a tool and the structure theorem for a maximal graph, we give a proof for our main result. In Section 4, from a symmetric analogue of Schwarz's rearrangement theorem, we single out a new equivalent condition for a threshold graph. In Section 5, we draw attention to the quasi-complete graphs and the quasi-stars, introduced by Ahlswede and Katona [2] in their study of the related problem of maximizing the number of adjacent pairs of edges of a graph with given numbers of vertices and edges, and pose an open question for the maximal Q-index problem. In Section 6, the final section, we rewrite a necessary condition for an optimal graph of the maximal index problem, which is implicit in Rowlinson's proof for the Brualdi–Hoffman conjecture, as a necessary condition for an optimal graph of the maximal index problem on connected graphs.

We would like to add that the present proof for the main result of this paper is different from the one as given in the thesis [9] of the first-named author, which was carried out by matrix block multiplication and was considerably longer. Also, unlike in our recent papers [10,28,11], in this work we do not make use of the concept of reduced graph matrices.

2. Preliminaries

The *line graph* L_G of a graph G is the graph whose vertices are the edges of G, with two vertices in L_G adjacent whenever the corresponding edges in G have exactly one vertex in common.

Let G be a graph with vertices $v_1, \ldots, v_n$ and edges $e_1, \ldots, e_m$. By the *vertex-edge incidence matrix* of G we mean the $n \times m$ matrix $M(G) = (m_{ij})$ given by: m_{ij} equals 1 if vertex v_i is on edge e_j and equals 0 otherwise. The following equality relations are well known: $Q(G) = M(G)M(G)^T$ and $2I_m + A(L_G) = M(G)^T M(G)$. From these relations, we obtain $q_1(G) = 2 + \rho(A(L_G))$, where $q_1(G)$ denotes the Q-index of G and $\rho(B)$ denotes the spectral radius of a square matrix B. It is also known that if x is the Perron vector of $Q(G)$ then $y := M(G)^T x$ is the Perron vector of $A(L_G)$ (see, for instance, [14, Section 4]). We index the components of x (respectively, of y) by the vertices (respectively, edges) of G. From the definition we have $y_{uv} = x_u + x_v$, where uv denotes the edge joining u and v.

It was announced in [14] and proved independently in [15,27] that every graph (respectively, connected graph) that maximizes the Q-index among all graphs (respectively, connected graphs) with fixed numbers of vertices and edges is a threshold graph (respectively, maximal graph). Here, following Merris [20], we call a graph (degree) *maximal* if it is connected and its degree sequence is not majorized by the degree sequence of other graph. Closely related to maximal graphs are threshold graphs, which are precisely graphs that are either maximal or are the (disjoint) union of a maximal graph and a null (i.e., edgeless) graph. There are many known equivalent conditions for a graph to be threshold (see [21,27]) and in the literature various other names have also been used for a threshold graph such as a nested split graph, a graph with a stepwise adjacency matrix, etc.

A square (0, 1)-matrix $A = [a_{ij}]$ is said to be *stepwise* (in its strictly upper triangular part) if it has the following property:

$$\text{If } i < j \text{ and } a_{ij} = 1, \text{ then } a_{hk} = 1 \text{ whenever } h < k \le j \text{ and } h \le i.$$

In the early study of the maximal index problem, the general case or the connected case, it was found that every optimal graph has a stepwise adjacency matrix [7, Theorem 2.1] and [8, Theorem 2.1]. This property of the optimal graph has played a role in the subsequent development.

For vertex-disjoint graphs G, H, we use $G \cup H$ to denote their (disjoint) *union*. For such pair of graphs, their *join*, $G \vee H$, is the graph obtained from $G \cup H$ by joining each vertex of G to every vertex of H.

For a vertex v of G, we denote by $d_G(v)$ and $N_G(v)$ respectively the *degree* and the *set of neighbors* of v in G. We denote the complement of G by G^c. The complete graph (respectively, null graph) on n vertices are written as K_n and K_n^c respectively. For convenience, we use K_0 or K_0^c to stand for the empty graph (i.e., one without vertices or edges) and adopt the convention that $G \cup K_0 = G$ and $G \vee K_0 = G$.

For a positive integer n, we use $\langle n \rangle$ to denote the set $\{1, \ldots, n\}$.

The concept of neighborhood equivalence classes of a graph and the structure theorem for a maximal graph will play a role in this work.

For a graph G, by the *neighborhood equivalence relation* (respectively, *vicinal pre-order*) on G we mean the equivalence relation $\sim^G$ (respectively, pre-order $\geq^G$) on $V(G)$ given by: $u \sim^G v$ if and only if $N_G(u) \setminus \{v\} = N_G(v) \setminus \{u\}$ (respectively, $u \geq^G v$ if and only if $N_G(u) \setminus \{v\} \supseteq N_G(v) \setminus \{u\}$). The equivalence classes for $\sim^G$ are called the *neighborhood equivalence classes* of G. In [27] the symbol $C(n_1, \ldots, n_r)$ is introduced to denote a maximal graph G with neighborhood equivalence classes $V_1, \ldots, V_r$, arranged in strict ascending order with respect to the total partial order on the quotient set $V(G)/\sim^G$ induced by the vicinal pre-order $\geq^G$ of G (or simply, with respect to $\geq^G$, by abuse of language) such that the cardinality of V_i is n_i, for $i = 1, \ldots, r$. It is readily shown that if δ_i denotes the common degree of vertices belonging to V_i, then $\delta_n > \delta_{n-1} > \cdots > \delta_1$. So for a maximal graph, the partition of the vertex set of the graph by its neighborhood equivalence classes and the degree partition are identical (see [27, p. 745] or [21, p. 9] for the definition of degree partition).

This work relies on the following structure theorem for a maximal graph, which describes completely how the edges link the various neighborhood equivalence classes, and whether an equivalence class is a clique or a stable set: if $V_1, \ldots, V_r$ are the neighborhood equivalence classes of a maximal graph G, arranged in strict ascending order with respect to $\geq^G$, then for any $i, j \in \langle r \rangle$, there exist edges between every vertex of V_i and every vertex of V_j (except when $i = j$ and V_i is a singleton) if $i + j \geq r + 1$, and there are no edges between vertices of V_i and vertices of V_j if $i + j < r + 1$ (see [27, Theorem 4.3]).

We also need the fact that if the vertices of a maximal graph G are arranged in non-increasing order of their degrees, then the components of the Perron vector x of $Q(G)$ are also in non-increasing order (see [27, Theorem 4.3]).

3. Proof for the main result

Proof of Theorem. Since a graph with maximal Q-index over all connected graphs with n vertices and $n + k$ edges is necessarily a maximal graph, it suffices to show that $q_1(H_{n,k}) > q_1(G)$ for every maximal graph G that has n vertices and $n + k$ edges and is different from $H_{n,k}$. For that matter, we need only show that $y^T A(L_{H_{n,k}})y - y^T A(L_G)y > 0$, where y is the Perron vector of $A(L_G)$, because once this is proved, it will follow that we have

$$\begin{aligned} q_1(H_{n,k}) &= 2 + \rho(A(L_{H_{n,k}})) \geq 2 + \frac{y^T A(L_{H_{n,k}})y}{\|y\|^2} \\ &> 2 + \frac{y^T A(L_G)y}{\|y\|^2} = 2 + \rho(A(L_G)) = q_1(G). \end{aligned}$$

We label the vertices of G and those of $H_{n,k}$ both by $v_1, \ldots, v_n$, arranged in non-increasing order of their vertex degrees. Note that G has precisely one dominating vertex, as $k \leq n - 3$ and $G \neq H_{n,k}$.

Let $G = C(n_1, \ldots, n_r)$, and let V_j be the neighborhood equivalence class with cardinality n_j for $j = 1, \ldots, r$. Denote by τ the largest index i such that v_i and v_{i+1} are adjacent in G. It is clear that V_r consists of $v_1, \ldots, v_{n_r}$, V_{r-1} consists of $v_{n_r+1}, v_{n_r+2}, \ldots, v_{n_r+n_{r-1}}$, and so forth. When r is even, by the structure theorem of a maximal graph, there are edges between $V_{\frac{r}{2}+1}$ and $V_{\frac{r}{2}}$, and $\cup_{j=1}^{\frac{r}{2}} V_j$ is a stable set. It follows that v_τ is the last element (i.e., the element with the largest index) of $V_{\frac{r}{2}+1}$, $d_G(v_{\tau+1}) = \tau$ and $v_{\tau+1}, \ldots, v_n$ form a stable set. Similarly, when r is odd, v_τ is the last but one element of $V_{\frac{r+1}{2}}$ and it is also true that $d_G(v_{\tau+1}) = \tau$ and $v_{\tau+1}, \ldots, v_n$ form a stable set. As $d_G(v_1) \geq d_G(v_2) \geq \cdots \geq d_G(v_{\tau+1}) = \tau$, there exist nonnegative integers s_i $(i = 1, \ldots, \tau)$ with $n - 1 - \tau = s_1 \geq s_2 \geq \cdots \geq s_\tau$ such that $d_G(v_i) = \tau + s_i$.

We are going to show that $\tau \geq 3$. If $\tau = 1$, then v_1 is a dominating vertex and $v_2, \ldots, v_n$ form a stable set. So G is the star $K_{1,n-1}$; hence $n + k = n - 1$ and we have $k = -1$, which is a contradiction. If $\tau = 2$, then v_2 is adjacent to v_3 and possibly also to other v_j's. In this case, $\{v_3, \ldots, v_n\}$ is a stable set. Hence G must be of the form $H_{p,q}$ for some nonnegative integers p, q. As a graph of such form and with given numbers of vertices and edges is unique, necessarily $G = H_{n,k}$, which is a contradiction.

Next, we show that $\tau + s_2 + 1 \geq 5$. Note that $G - v_1$ is a threshold graph with $k + 1$ edges, and as $k + 1 \geq 4$ the nontrivial component of $G - v_1$ has at least four vertices. But v_2 is a dominating vertex of the nontrivial component of $G - v_1$, so $d_G(v_2) = 1 + d_{G-v_1}(v_2) \geq 4$ and we have $\tau + s_2 + 1 = d_G(v_2) + 1 \geq 5$.

In what follows we take $y = M(G)^T x$, where x is the Perron vector of $Q(G)$.

For brevity, write the edge $v_i v_j$ of G (also, of $H_{n,k}$) as $e_{i,j}$, always assuming that $i < j$. Arrange the edges of G (also, of $H_{n,k}$) in the lexicographic ordering, i.e., in the order $e_{1,2}, e_{1,3}, \ldots, e_{1,n-1}, e_{2,3}, e_{2,4}$, etc. Index the rows and columns of $A(L_G)$ (respectively, of $A(L_{H_{n,k}})$) by the edges of G (respectively, by the edges of $H_{n,k}$). When evaluating $y^TA(L_G)y$, we index the components of y by the edges of G. In this case, for any edge $e_{r,s}$ of G, we have $y_{e_{r,s}} = x_r + x_s$. On the other hand, when evaluating $y^TA(L_{H_{n,k}})y$, we index the components of y by the edges of $H_{n,k}$. In this case, we set up a one-to-one correspondence between $E(H_{n,k}) \setminus E(G)$ and $E(G) \setminus E(H_{n,k})$ (in an arbitrary manner). For $e_{i,j} \in E(H_{n,k}) \cap E(G)$, we take $y_{e_{i,j}} = x_i + x_j$. For $e_{i,j} \in E(H_{n,k}) \setminus E(G)$, $y_{e_{i,j}}$ is taken to be $x_r + x_s$, where $e_{r,s}$ is the edge in $E(G) \setminus E(H_{n,k})$ that corresponds to $e_{i,j}$ in the above correspondence.

Let $\mathcal{E}$ denote the set of edges of G of the form $e_{i,j}$ with $i \geq 3$. To obtain $H_{n,k}$ from G, we add the edges $e_{2,j}$ for $j = \tau + 2 + s_2, \ldots, k+3$, and delete the edges that belong to $\mathcal{E}$. As a result, we create the following new pairs of adjacent edges:

$$\{e_{1,2}, e_{2,j}\}, \{e_{1,j}, e_{2,j}\}, \{e_{2,3}, e_{2,j}\}, \ldots, \{e_{2,\tau+1+s_2}, e_{2,j}\} \text{ for } j = \tau + 2 + s_2, \ldots, k+3;$$

$$\{e_{2,i}, e_{2,j}\} \text{ for } \tau + 2 + s_2 \leq i < j \leq k+3,$$

and remove the following old pairs of adjacent edges:

$$\{e_{1,r}, e_{r,s}\}, \{e_{1,s}, e_{r,s}\}, \{e_{2,r}, e_{r,s}\}, \{e_{2,s}, e_{r,s}\} \text{ for } e_{r,s} \in \mathcal{E};$$

$$\{e_{i,j}, e_{r,s}\} \text{ for } e_{i,j}, e_{r,s} \in \mathcal{E} \text{ such that } |\{i,j\} \cap \{r,s\}| = 1.$$

So we have

$$\frac{1}{2}[y^TA(L_{H_{n,k}})y - y^TA(L_G)y] = \sum_{\{e,f\} \in E(L_{H_{n,k}})} y_e y_f - \sum_{\{e,f\} \in E(L_G)} y_e y_f = \sigma_1 - \sigma_2,$$

where

$$\sigma_1 = \sum_{j=\tau+s_2+2}^{k+3} y_{e_{2,j}} \left(y_{e_{1,2}} + y_{e_{1,j}} + \sum_{i=3}^{\tau+1+s_2} y_{e_{2,i}} \right) + \sum_{\tau+2+s_2 \leq i < j \leq k+3} y_{e_{2,i}} y_{e_{2,j}}$$

and

$$\sigma_2 = \sum_{e_{r,s} \in \mathcal{E}} \left(y_{e_{1,r}} + y_{e_{1,s}} + y_{e_{2,r}} + y_{e_{2,s}} \right) y_{e_{r,s}} + \sum y_{e_{i,j}} y_{e_{r,s}},$$

where the last sum in σ_2 is taken over all possible (unordered) pairs of adjacent edges e_{ij}, e_{rs} of G that belong to $\mathcal{E}$. Since $\{y_{e_{2,i}} : i = \tau + 2 + s_2, \ldots, k+3\} = \{y_{e_{r,s}} : e_{r,s} \in \mathcal{E}\}$, it is clear that the last sum in σ_2 is less than or equal to the last sum in σ_1. So we have

$$\sigma_1 - \sigma_2 \geq \sum_{j=\tau+s_2+2}^{k+3} y_{e_{2,j}} \left(y_{e_{1,2}} + y_{e_{1,j}} + \sum_{i=3}^{\tau+1+s_2} y_{e_{2,i}} \right) - \sum_{e_{r,s} \in \mathcal{E}} (y_{e_{1,r}} + y_{e_{1,s}} + y_{e_{2,r}} + y_{e_{2,s}}) y_{e_{r,s}}.$$

Consider any fixed j, $\tau + 2 + s_2 \leq j \leq k+3$. There exists a unique $e_{r,s} \in \mathcal{E}$ such that $y_{e_{2,j}} = y_{e_{r,s}}$. Since $\tau + 1 + s_2 \geq 5$, we have

$$\begin{aligned}
&\left(y_{e_{1,2}} + y_{e_{1,j}} + \sum_{i=3}^{\tau+1+s_2} y_{e_{2,i}} \right) - (y_{e_{1,r}} + y_{e_{1,s}} + y_{e_{2,r}} + y_{e_{2,s}}) \\
&\geq (y_{e_{1,2}} + y_{e_{1,j}} + y_{e_{2,3}} + y_{e_{2,4}} + y_{e_{2,5}}) - (y_{e_{1,r}} + y_{e_{1,s}} + y_{e_{2,r}} + y_{e_{2,s}}) \\
&= (x_1 + x_2) + (x_1 + x_j) + (x_2 + x_3) + (x_2 + x_4) + (x_2 + x_5) - (x_1 + x_r) \\
&\quad -(x_1 + x_s) - (x_2 + x_r) - (x_2 + x_s) \\
&= (x_2 - x_r) + (x_2 - x_r) + (x_3 - x_s) + (x_4 - x_s) + x_j + x_5 > 0,
\end{aligned}$$

where the last inequality follows from the fact that the components of the Perron vector x are arranged in non-increasing order. This establishes $\sigma_1 - \sigma_2 > 0$, as desired. $\square$

A close examination of the above proof shows that the quantity τ that appears in the proof is given by:

$$\tau = \delta_{\lceil \frac{r}{2} \rceil} = \begin{cases} n_r + n_{r-1} + \cdots + n_{\frac{r}{2}+1} & \text{when } r \text{ is even} \\ n_r + n_{r-1} + \cdots + n_{\frac{r+1}{2}} - 1 & \text{when } r \text{ is odd,} \end{cases}$$

where δ_j denotes the common degree of the vertices belonging to V_j. In fact, $\tau + 1$ is equal to the clique number of G, and τ is what some people call the *trace of the degree sequence* of G or, equivalently, the number of boxes on the main diagonal of the Ferrers-Sylvester diagram for the degree sequence of G (cf. [27, Remark 7.4]).

4. A new equivalent condition for a threshold graph

The following is a symmetric analogue of Schwarz's rearrangement theorem. It is probably known (see [7, the paragraph preceding Theorem 2.1]) and is not difficult to prove.

Theorem 4.1. *If* $(n^2 - n)/2$ *nonnegative numbers are given, then the largest spectral radius of an* $n \times n$ *real symmetric matrix which has zero trace and whose entries above the diagonal are these given numbers can be found among those matrices where the off-diagonal entries in each row* (*and each column*) *are non-increasing.*

By applying the preceding theorem to the adjacency matrix of a graph, one can see that if G has maximal index among all graphs with n vertices and m edges then the following holds:

> G has an adjacency matrix with the property that in each row the 1's are to the left of the off-diagonal 0's.

The above property of a graph G is actually a variant of the property that G has a stepwise adjacency matrix. What is true in general is the following:

Lemma 4.2. *For any symmetric* $(0, 1)$*-matrix A, the following conditions are equivalent*:

(a) *The matrix A is stepwise.*
(b) *In each row of A, the* 1*'s are to the left of the off-diagonal* 0*'s.*

Proof. First, note that for any square $(0, 1)$-matrix A, condition (a) is equivalent to the following apparently weaker (and simpler) condition:

(a$'$) If $a_{ij} = 1$ and $i < j$ then $a_{ik} = 1$ whenever $i + 1 \le k < j$ and $a_{lj} = 1$ whenever $1 \le l < i$.

Also, condition (b) can be rewritten as:

(b$'$) For each i, if $a_{ij} = 1$ then $a_{ik} = 1$ for all $k < j$, $k \neq i$.

Now using the fact that A is symmetric, it is not difficult to show that conditions (a$'$) and (b$'$) are equivalent, hence so are conditions (a) and (b). $\square$

As noted before, every optimal graph for the maximal Q-index problem over connected graphs is a maximal graph and hence a threshold graph. We believe it is a known fact that a graph is threshold if and only if the graph has a stepwise adjacency matrix, but we are unable to find in the literature an explicit statement with a proof for this fact. For completeness, in below we give a proof.

Lemma 4.3. *Let G be a graph.*

(i) *If G is a threshold graph and if the vertices $v_1, \ldots, v_n$ of G are arranged in non-increasing order of their vertex degrees, then the adjacency matrix A of G satisfies the equivalent conditions of Lemma 4.2.*

(ii) *If G has an adjacency matrix that satisfies the equivalent conditions of Lemma 4.2, then G is threshold.*

Proof. An equivalent condition for G to be threshold (see [27, Section 4]) is that the vicinal pre-order of G is total, i.e., for any vertices v_1, v_2 of G, we have, either $N_G(v_1) \setminus \{v_2\} \subseteq N_G(v_2) \setminus \{v_1\}$ or $N_G(v_2) \setminus \{v_1\} \subseteq N_G(v_1) \setminus \{v_2\}$. We will make use of the above equivalent condition as well as the following variant of it:

For any vertices v_1, v_2 of G, if $d_G(v_1) \leq d_G(v_2)$ then $N_G(v_1) \setminus \{v_2\} \subseteq N_G(v_2) \setminus \{v_1\}$.

(i) Suppose that $a_{ij} = 1$. Consider any $k \neq i$, $k < j$. Since $d_G(v_k) \geq d_G(v_j)$ and G is threshold, we have $N_G(v_k) \setminus \{v_j\} \supseteq N_G(v_j) \setminus \{v_k\}$. As $v_i \in N_G(v_j) \setminus \{v_k\}$, it follows that $v_i \in N_G(v_k)$ and hence $a_{ik} = 1$. This proves that in each row of A the 1's precede the off-diagonal 0's.

(ii) Suppose that G has an adjacency matrix A that satisfies the equivalent conditions of Lemma 4.2. For each i, let $l(i)$ denote the largest index j such that $a_{ij} = 1$. We contend that $l(1) \geq l(2) \geq \cdots \geq l(n)$. Assume to the contrary that there exists i such that $l(i) < l(i+1)$. Then we have $a_{i+1,\, l(i+1)} = 1$ and $a_{i,\, l(i+1)} = 0$. Furthermore, $l(i+1) \neq i$; else, we have $a_{i,i+1} = a_{i+1,i} = 1$ and so $l(i) \geq i+1 > i = l(i+1)$, which is a contradiction. So in the $l(i+1)$th column, and hence in the $l(i+1)$th row, of A it is not true that the 1's precede the off-diagonal 0's. Thus we arrive at a contradiction.

Now let τ be the largest index i such that $a_{i,i+1} = 1$. Then $l(\tau+1) = \tau$ and we have

$$N_G(v_i) = \begin{cases} \{v_1, \ldots, v_{l(i)}\} \setminus \{v_i\} & \text{for } i \leq \tau \\ \{v_1, \ldots, v_{l(i)}\} & \text{for } i \geq \tau+1 \end{cases}.$$

Consider any pair of distinct indices $i, j \in \langle n \rangle$, $i < j$. By treating the three cases $\tau \geq j > i$, $j > \tau \geq i$ and $j > i \geq \tau + 1$ separately, we obtain

$$N(v_i) \setminus \{v_j\} = \{v_1, \ldots, v_{l(i)}\} \setminus \{v_i, v_j\} \text{ and } N(v_j) \setminus \{v_i\} = \{v_1, \ldots, v_{l(j)}\} \setminus \{v_i, v_j\}.$$

Since $l(i) \geq l(j)$, the inclusion $N(v_i) \setminus \{v_j\} \supseteq N(v_j) \setminus \{v_i\}$ follows. This shows that the vicinal pre-order of G is total, and so G is a threshold graph. □

In view of Theorem 4.1 and Lemma 4.3, one may attribute to Schwarz the result that graphs with maximal index among all graphs with given numbers of vertices and edges are threshold graphs.

5. Quasi-complete graphs and quasi-stars

In all known cases of the maximal index problem for the class of connected graphs, a connected graph with maximal index is one of two types $H_{n,k}$ (defined for $-1 \leq k \leq n-3$ only) and $G_{n,k}$ (defined for $-1 \leq k \leq \binom{n}{2} - n$). The graph $H_{n,k}$ has already been defined. To define $G_{n,k}$, first write $k+1$ as $\binom{d}{2} + s$, where $0 \leq s \leq d-1$. The graph $G_{n,k}$ has a spanning star with $n-1$ edges, and the remaining $k+1$ edges form a complete graph on d vertices plus s edges from another vertex to s vertices of the complete graph.

For further investigation on the maximal index problem on connected graphs or the maximal Q-index problem (on graphs or connected graphs), it is worth looking at the quasi-complete graphs and the quasi-stars introduced by Ahlswede and Katona [2] in their study of the related (but easier) problem of determining graphs that maximize the number of adjacent pairs of edges (equivalently, the number of length-2 paths) among graphs with given numbers of vertices and edges.

The *quasi-complete graph* C_n^m and the *quasi-star* S_n^m both have n vertices and m edges. To construct C_n^m, write m as $\binom{a}{2} + b$ with $0 \le b < a$. The graph C_n^m is obtained by first joining b vertices of the complete graph K_a to a new vertex (when $b = 0$, just take K_a) and then taking (disjoint) union with the null graph K_{n-a-1}^c (with K_{n-a}^c in case $b = 0$). Note that C_n^m is always a threshold graph, and also that either one of the following two conditions is equivalent to the condition that C_n^m is a maximal graph: (1) $\binom{n-1}{2} + 1 \le m \le \binom{n}{2}$; (2) $C_n^m = G_{n,k}$ with $k = m - n$.

We use the representation $\binom{n}{2} - m = \binom{p}{2} + q$, where $0 \le q < p$, to construct S_n^m as follows: Form the star $K_{1,p-q}$, take the union with the null graph K_q^c and then take the join with the complete graph K_{n-p-1}; that is $S_n^m = (K_{1,p-q} \cup K_q^c) \vee K_{n-p-1}$. As can be readily checked, S_n^m is the complement of $C_n^{\binom{n}{2}-m}$. For $m \ge n-1$, S_n^m is always a maximal graph. But for $1 \le m \le n-2$, we have, $p = n-1$, $q = n-1-m > 0$, in which case K_{n-p-1} is the empty graph and S_n^m is the disconnected threshold graph $K_{1,m} \cup K_{n-1-m}^c$. Also, for $n-1 \le m \le 2n-3$, we have $S_n^m = H_{n,k}$ with $k = m-n$, as $\binom{n}{2} - m = \binom{n-2}{2} + (2n-3-m)$ and $0 \le 2n-3-m < n-2$ (with a slight modification in the argument in case $m = n-1$). Moreover, we also have

$$C_n^{\binom{n}{2}} = S_n^{\binom{n}{2}} = G_{n,\binom{n-1}{2}-1} = K_n.$$

The above-mentioned Brualdi–Hoffman conjecture, which Rowlinson has established, states that *for every pair of positive integers m, n with $m \le \binom{n}{2}$, the quasi-complete graph C_n^m is the unique graph that maximizes the index over all graphs with n vertices and m edges.*

Ahlswede and Katona have proved that one of the two graphs C_n^m and S_n^m always yields an optimal graph for their problem; in particular, S_n^m is an optimal graph for $0 \le m < \frac{1}{2}\binom{n}{2} - \frac{n}{2}$ and C_n^m is an optimal graph for $\frac{1}{2}\binom{n}{2} + \frac{n}{2} < m \le \binom{n}{2}$ (see [2, Theorem 2 and Theorem 3]).

Later Boesch et al. [6, Theorem 1.2] proved that optimal graphs for the length-2 paths problem are threshold graphs. By elaborating the arguments of [6], the first-named author has shown in her thesis [9, Theorem 6.3.2] that optimal graphs for the length-2 paths problem over connected graphs are maximal graphs, and also she has made the following observation (which undoubtedly is, at least, partly known):

Remark 5.1. For graphs (or connected graphs) with given numbers of vertices and edges, the problems of maximizing any one of the following quantities are equivalent: the number of adjacent pairs of edges, the number of length 2-paths, the number of edges in the line graph, sum of squares of vertex degrees, the Frobenius norm of the signless Laplacian, and the sum of the entries of the square of the adjacency matrix.

Besides the above-mentioned Schwarz's rearrangement theorem, in [25] the following is also proved: *if n^2 nonnegative real numbers (not necessarily pairwise distinct) are given, then among the $n \times n$ matrices whose entries are these given numbers it is possible to find one, where the entries in each row and each column are non-increasing, such that the sum of the entries of the square of the matrix attains the maximum.*

In view of Remark 5.1, one may say that the work in Schwarz's paper [25] has anticipated much of the later developments on (0, 1)-matrices or on graphs: for instance, the above-mentioned work of Boesch, etc. on the length-2 paths problem (see [6]), Aharoni's work on maximal sum of the elements of A^2 for an $n \times n$ (0, 1)-matrix A with given number of 1's (see [1]), and Nikiforov's work on the maximum of the sum of the squares of degrees of a graph with given numbers of vertices and edges (see [22]), etc.

In related to the maximal Q-index problem, we would like to pose the following question:

Question. Is it true that for every pair of positive integers m, n, with $m \le \binom{n}{2}$, one of the two graphs S_n^m or C_n^m maximizes the Q-index over all graphs with n vertices and m edges?

Note that the problem of maximizing the Q-index over all connected graphs with m edges and at most n vertices is equivalent to the problem of maximizing the Q-index over all (not necessarily connected) graphs with m edges and n (or at most n) vertices.

An affirmative answer to the above question is supported by the following results obtained in [11, Theorem 6.1(b)] and [10, Theorems 4.6–4.9] but slightly reformulated here.

Theorem 5.2. *For $m \geq 4$, $n \geq m+1$, S_n^m $(= K_{1,m} \cup K_{n-m-1}^c)$ is the unique graph with maximal Q-index among all graphs with n vertices and m edges.*

Theorem 5.3. *For every positive integer $m \geq 4$, S_m^m (with $S_4^4 = C_4^4$ for $m = 4$) is the unique graph with maximal Q-index among all graphs with m edges and m vertices.*

Theorem 5.4. *For $m \geq 5$, there is a unique graph with maximal Q-index among all graphs with m edges and $m-1$ vertices: for $m = 5$ (respectively, $m = 6$, $m \geq 7$), the optimal graph is $S_4^5 (= C_4^5)$ (respectively, $C_5^6 (= K_4 \cup K_1^c)$, S_{m-1}^m).*

Theorem 5.5. *For $m \geq 7$, there are precisely two graphs that have maximal Q-index among all graphs with m edges and $m-2$ vertices, namely, S_{m-2}^m and $G_{m-2,2}$.*

Theorem 5.6. *For $m \geq 8$, except $m = 10$, there is a unique graph with maximal Q-index among all graphs with m edges and $m-3$ vertices, namely, S_{m-3}^m. For $m = 10$, there are two optimal graphs, namely, $C_7^{10} (= K_5 \cup K_2^c)$ and S_7^{10}.*

6. A necessary condition for the maximal index problem

In the course of establishing the Brualid–Hoffman conjecture, Rowlinson [24, Lemma 2] has showed the following:

Remark 6.1. If the adjacency matrix $A(G) = (a_{ij})_{1 \leq i,j \leq n}$ of a graph G is stepwise and for some indices $h, k, p, q \in \langle n \rangle$ we have

(i) $h < p < q < k$;
(ii) $a_{hk} = 1$, $a_{hj} = 0$ whenever $j > k$, $a_{ik} = 0$ whenever $i > h$;
(iii) $a_{pq} = 0$, $a_{pj} = 1$ whenever $p < j < q$, $a_{iq} = 1$ whenever $i < p$;
(iv) $p + q > h + k + 1$,

then $\rho(A(G)) < \rho(A(G'))$, where G' is the graph obtained from G by replacing the edge $v_h v_k$ by $v_p v_q$.

We take this opportunity to rewrite the above observation as a necessary condition for the optimal graph of the maximal index problem over connected graphs.

Theorem 6.2. *Let G be a maximal graph with maximal index among all connected graphs with given numbers of vertices and edges. Let $\delta_r > \cdots > \delta_1$ be the distinct vertex degrees of G. Then for every pair of indices $i, l \in \langle r \rangle$, $\lfloor \frac{r-1}{2} \rfloor \geq l > i$ (and in case $i = 1$ we require that G has at least two dominating vertices), we have, $\delta_i + \delta_{r+1-i} \geq \delta_l + \delta_{r-l} + 1$.*

Proof. Let $V_1, \ldots, V_r$ be the neighborhood equivalence classes of G, arranged in strict ascending order with respect to $\geq^G$. Clearly, vertices in V_i share the common degree δ_i for $i = 1, \ldots, r$.

Let n_i denote the cardinality of V_i for $i = 1, \ldots, r$, and arrange the vertices of G in non-increasing order of their vertex degrees. By Lemma 4.3(i) the adjacency matrix $A(G) = (a_{st})$ of G is stepwise.

Consider any pair of indices $i, l \in \langle r \rangle$, $\lfloor \frac{r-1}{2} \rfloor \geq l > i$. Let v_k be the last vertex in V_i, v_h be the last vertex in V_{r+1-i}, v_q be the first vertex in V_l and v_p be the first vertex in V_{r-l}. It is readily shown that we have $r+1-i > r-l > l > i$ and hence $h < p < q < k$. Since $v_k \in V_i$ and $v_h \in V_{r+1-i}$, by the property of a maximal graph mentioned at the beginning, we have $a_{hk} = 1$. As v_k is the last vertex in V_i, for every $t > k$, we have $v_t \in V_1 \cup \cdots \cup V_{i-1}$ and so $a_{ht} = 0$. Similarly, we also have $a_{sk} = 0$ whenever $s > h$. So conditions (i), (ii) of Remark 6.1 are satisfied. Similarly, we can also verify condition (iii).

Since v_k is the last vertex in V_i, we have

$$k = n_r + n_{r-1} + \cdots + n_i = \delta_{r+1-i} + 1.$$

Similarly, we have

$$h = n_r + n_{r-1} + \cdots + n_{r+1-i} = \delta_i,$$

$$q = n_r + n_{r-1} + \cdots + n_{l+1} + 1 = \delta_{r-l} + 2,$$

and

$$p = n_r + n_{r-l} + \cdots + n_{r-l+1} + 1 = \delta_l + 1.$$

It follows that the desired inequality $\delta_i + \delta_{r+1-i} \geq \delta_l + \delta_{r-l} + 1$ is equivalent to $p + q \leq h + k + 1$. If the desired inequality does not hold, then by Remark 6.1 we have $\rho(A(G)) < \rho(A(G'))$, where $G' = G - v_h v_k + v_p v_q$. But G' is a connected graph — because it has a dominating vertex — with the same number of vertices and edges as G, so we arrive at a contradiction. □

In Theorem 6.2 one may replace the condition $l > i$ by $l \geq i$ by including the trivial case $l = i$.

It is of interest to compare the above result with the following known result [10, Theorem 3.10] for the signless Laplacian.

Theorem 6.3. *Let G be a maximal graph that maximizes the Q-index among all connected graphs with fixed numbers of vertices and edges. Let $\delta_r > \delta_{r-1} > \cdots > \delta_1$ be the distinct vertex-degrees of G. Then $\delta_i + \delta_{r+1-i} \geq \delta_l + \delta_{r-l} + 2$ for every pair of positive integers i, l that satisfy $l + 2 \leq i \leq \lceil \frac{r}{2} \rceil$.*

We are not sure whether Theorem 6.2 (respectively, Theorem 6.3) can be useful at all in the future study of the maximal index (respectively, Q-index) problem over connected graphs. Note that the existence of positive integers i, l such that $\lfloor \frac{r-1}{2} \rfloor \geq l > i$ (or $l+2 \leq i \leq \lceil \frac{r}{2} \rceil$) implies that $r \geq 5$. The maximal graph $H_{n,k}$ can have one, two, three or four neighborhood equivalence classes, depending on n and k. So neither Theorem 6.2 nor Theorem 6.3 can be applied to $H_{n,k}$ non-vacuously. The maximal graph $G_{n,k}$ can have one up to five neighborhood equivalence classes: it is when $k+1 = \binom{d}{2} + s$ with $1 \leq s \leq d-2$, $d < n-2$, that $G_{n,k}$ has five neighborhood equivalence classes, and in that case $G_{n,k} = C(n-d-2, 1, d-s, s, 1)$. So Theorem 6.2 cannot be applied to $G_{n,k}$ non-vacuously; and Theorem 6.3 can be applied non-vacuously to $G_{n,k}$ only when $G_{n,k}$ is of the form $G_{n,k} = C(n-d-2, 1, d-s, s, 1)$, but that is the one-dominating-vertex case of the maximal Q-index problem over connected graphs, for which we have already had a complete answer: $H_{n,k}$ is the unique optimal graph, according to the main result of this paper. As for the maximal graph S_n^m (with $m \geq n-1$), again neither Theorem 6.2 nor Theorem 6.3 can be applied non-vacuously, as S_n^m has at most four neighborhood equivalence classes.

It is likely that every optimal graph for the index problem or Q-index problem over connected graphs has at most five neighborhood equivalence classes. By [10, Corollary 3.11], we have established only the following very modest result: for the Q-index problem over connected graphs, the number of neighborhood equivalence classes of an optimal graph is always less than or equal to four-fifth of its number of vertices.

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